NASA Unified Weather Research and Forecasting Model (NU-WRF)

A Tutorial

For Bjerknes Patch 5

NUWRF software integration group

September 22, 2017

Introduction

What is in this tutorial?

This tutorial describes the process of downloading, compiling, and running NU-WRF (Bjerknes patch 5 release) for five different and representative workflows:

- Basic: Based on WRF ARW.
- WRF-LIS: The recommended non-chemistry NU-WRF workflow (LIS MERRA forcing).
- WRF-LIS: The recommended non-chemistry NU-WRF workflow (LIS NLDAS2 forcing).
- Chemistry: The recommended chemistry (non-LIS) NU-WRF workflow.
- SCM: The Single Column Model NU-WRF workflow.

Each workflow consists of a series of steps starting with the acquisition of data files followed by the execution of several NU-WRF components. Successful completion of any workflow requires that **all** steps be completed in the order presented.
For any additional information please consult the NU-WRF user's guide at:
https://nuwrf.gsfc.nasa.gov/sites/default/files/docs/nuwrf_userguide.pdf

Special instructions

- All workflows are designed with pre-defined settings[1], including datasets. So, please refrain from editing the inputs unless you know what you are doing.
- It is assumed that users are running on Discover or Pleiades[2], using the bash shell. However, the steps described here *should* work under other shells

IMPORTANT: All lines starting with '>' are Unix commands to be executed by the users.

[1] That is, compiler/MPI combination, external libraries and run-time settings.

[2] Only the basic workflow is available on Pleiades.

Useful links

- Community ARW User Guide
  http://www2.mmm.ucar.edu/wrf/users/docs/user_guide_V3.5/contents.html
- Community WRF ARW Online Tutorial
  http://www2.mmm.ucar.edu/wrf/OnLineTutorial/index.htm
- Documentation for using Discover and other NCCS systems
  http://www.nccs.nasa.gov/primer/
- Documentation for using Pleiades and other NAS systems
  http://www.nas.nasa.gov/hecc/support/kb/161/

NOTE: The details for building the software on Discover and Pleiades are automatically handled by NUWRF's build scripts!

Setup

Before starting any workflow there are a few steps that must be completed:

- Download or checkout the NU-WRF code.
- Build the NU-WRF executable components.
- Set some environment variables.

Download the code

Tar files are available to NCCS and NAS s0942 group members.
On DISCOVER:

```
> cp /discover/nobackup/projects/nu-wrf/releases/stable/<tarball>
     /some/path
where tarball is:
nu-wrf_v8p5-wrf371-lis72r.tar.gz
```

On PLEIADES:

```
> cp /nobackupp8/nuwrf/releases/stable/<tarball> /some/path
where tarball is:
nu-wrf_v8p5-wrf371-lis72r.tar.gz
```

To untar type:

```
> tar -zxf nu-wrf_v8p4-wrf371-lis71rp7.tar.gz
```

Download the code

Developers can clone the code from the GIT repository. For example:

```
\begin{lstlisting}
> cd /discover/nobackup/user_id/
> git clone progressdirect:/git/projects/nu-wrf
```

For more information refer to the NU-WRF user's guide:

```
https://nuwrf.gsfc.nasa.gov/sites/default/files/docs/
    nuwrf_userguide.pdf
```

Build NU-WRF

First log in to a Discover SP3 node or Pleiades front end node.
Create environment variable **NUWRFDIR** that defines directory path of NU-WRF code downloaded earlier. Then, **cd** to it. For example, on Discover:

```
> export NUWRFDIR=/discover/nobackup/user_id/nu-wrf
> cd $NUWRFDIR
```

Now execute the build script as follows (runs in background, saves output in make.log):
Basic workflow:

```
> ./build.sh wrf wps >& log.out &
```

WRF-LIS workflows:

```
> ./build.sh wrf wps lis ldt lisconfig >& log.out &
```

Chemistry workflow:

```
> ./build.sh chem wps utils >& log.out &
```

SCM workflow:

```
> ./build.sh ideal_scm_lis_xy wps lis ldt lis4scm >& log.out &
```

Build NU-WRF

After compilation - assuming there are no errors - several executables will be created. For example:

```
WRF executables:

$NUWRFDIR/WRFV3/main/real.exe
$NUWRFDIR/WRFV3/main/wrf.exe

WPS executables:

$NUWRFDIR/WPS/geogrid.exe
$NUWRFDIR/WPS/metgrid.exe
$NUWRFDIR/WPS/ungrib.exe
```

For example, to see the names of all the executables created with an exe extension run:

```
> find $NUWRFDIR -name \*.exe
```

Environment variables

We already set **NUWRFDIR** , but we need two more variables.

- Select a directory for running the model and set it equal to the **RUNDIR** environment variable. For example:

```
> export RUNDIR=/discover/nobackup/user_id/scratch/
    basic_workflow
```

- Make sure you create **RUNDIR** outside of **NUWRFDIR**.This is useful when switching between NU-WRF versions or for updating to new changes.
- Finally, set the **PROJECTDIR** environment variable:

```
> export PROJECTDIR=/discover/nobackup/projects/nu-wrf
```

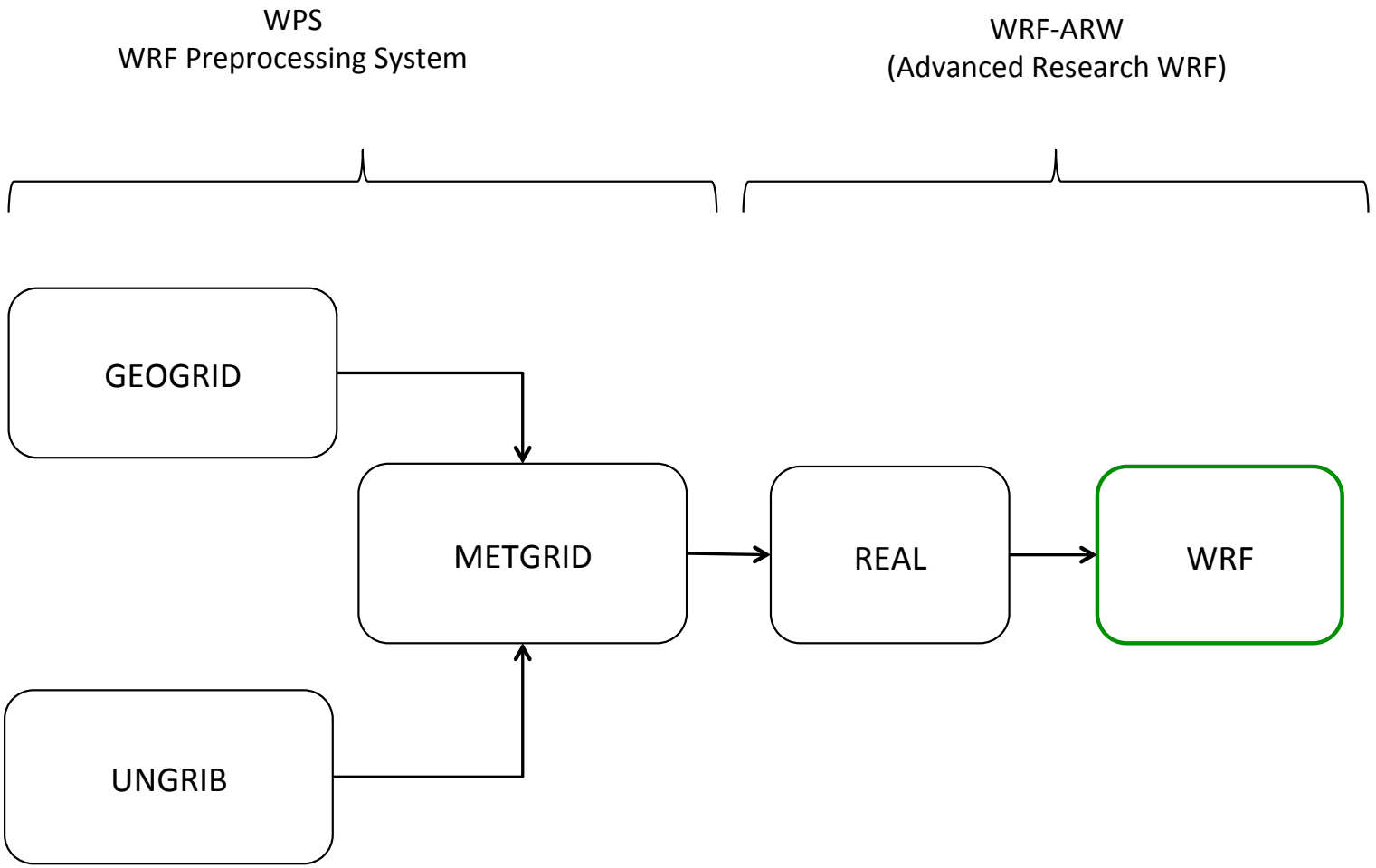
Please note that these variables (NUWRFDIR, RUNDIR, PROJECTDIR) are used in all workflows.

Basic Workflow

A NU-WRF workflow consists of running various pre-processing (WPS) components as well as the main NU-WRF model. The basic workflow described next is the simplest approach to running simulations with NU-WRF. It consists of running the WRF Pre-processing System (WPS) plus an additional WRF pre-processor (REAL) before running the WRF model.

Neither chemistry nor advanced land surface initialization are used.

NU-WRF basic workflow (similar to WRF ARW).



Required files for basic workflow

Copy the following files to **RUNDIR**:

```
> cp -r $PROJECTDIR/tutorial/basic $RUNDIR
```

```
Where:
common.cfg : shared script with settings used by other scripts.
run*.bash : scripts to run pre-processors and model.
namelist* : namelist files required by executables.
data/ungrib/* : GRIB atmospheric data for initial conditions used
     by UNGRIB component.
```

Required script changes

```
> cd $RUNDIR
```

Use your favorite editor to edit **common.cfg** and change the values of NUWRFDIR and RUNDIR using the values set earlier.

```
# *** Please make sure these settings are correct ***
# NUWRFDIR specifies the location of the NU-WRF source code
NUWRFDIR=<CHANGE THIS>
# RUNDIR specifies the location of the temporary run directory
RUNDIR=<CHANGE THIS>
```

You may need to edit all the run* files' account information and other settings. However, if you belong to group s0492 then the scripts should work without any modifications.

```
Change account to appropriate SBU charge code:
#SBATCH --account s0942
Change if you want to change number of nodes, hasw - to run on haswell nodes:
#SBATCH --ntasks=16 --constraint=hasw
Uncomment and set according to your needs and privileges:
##SBATCH --qos=high
Uncomment (if desired) and substitute your e-mail here:
##SBATCH --mail-user=user@nasa.gov
```

A note about namelists settings

Things to keep in mind before we run NU-WRF components.

- The length of the simulations is specified in the namelist files:
  - In namelist.wps the length is determined by start_date and end_date
  - In namelist.input look for start_ and end_ fields.
  - The dates in both namelists must be consistent.
- The workflow is designed to work as-is. However, if you want to run for different dates:
  - You must get the corresponding atmospheric data for initial conditions.
  - Yo may need to modify the namelists. For example in namelist.input, make sure end_day - start_day = run_days.
- For **any** other changes please refer to the user's guide.

GEOGRID

GEOGRID interpolates static and climatological terrestrial data (land use, albedo, vegetation greenness, etc) to each WRF grid.

- Input: namelist.wps
- Output: For *N* domains (max_dom in namelist.wps), *N* geo_em files will be created.

To run:

```
> cd $RUNDIR
> sbatch run_geogrid.bash
---
When done, check for "Successful completion" string in the file
    geogrid.slurm.out. geogrid.log.<node> will also be created
    for tracking run failures or debugging.
```

UNGRIB

UNGRIB reads GRIB or GRIB2 files with dynamic meteorological and dynamic terrestrial data (soil moisture, soil temperature, sea surface temperature, sea ice, etc) and writes specific fields in a WPS intermediate format.

- Input: namelist.wps and GRIB input data.
- Output: Several FNL* files corresponding to number of intervals (interval_seconds) in simulation length (start/end dates).

NOTE: The GRIB input is referenced in the run script, run_ungrib.bash:
./link_grib.csh data/ungrib/fnl_*
The UNGRIB output (FNL) is determined by the settings in the WPS namelist (namelist.wps).

To run:

```
> cd $RUNDIR
> ./run_ungrib.bash
or
> sbatch run_ungrib.bash
---
When done, check for "Successful completion" string in file
    ungrib_logs/ungrib.log.
```

METGRID

METGRID horizontally interpolates the output from UNGRIB to the WRF domains, and combines it with the output from GEOGRID.

- Input: namelist.wps, UNGRIB output, geo_em* files.
- Output: Several met_em* files corresponding to number of intervals (interval_seconds) in simulation length (start/end dates).

To run:

```
> cd $RUNDIR
> sbatch run_metgrid.bash
---
When done, check for "Successful completion" string in the file
    metgrid.slurm.out. metgrid.log.<node> will also be created
    for tracking run failures or debugging.
```

REAL

REAL vertically interpolates the METGRID output to the WRF grid, and creates initial and lateral boundary condition files.

- Input: namelist.input, met_em* files, geo_em* files.
- Output: wrfinput* files (one for each domain), wrfbdy_d01.

To run:

```
> cd $RUNDIR
> sbatch run_real.bash
---
Check real.slurm.out for run completion.
Also check real.rsl.out.<node> and real.rsl.error.<node> for
    tracking run failures or debugging.
```

WRF

This program will perform a numerical weather prediction simulation using the data from REAL.

- Input: wrfinput* files (one for each domain), wrfbdy_d01.
- Output: wrfout* and wrfrst* files (one for each domain).

To run:

```
> cd $RUNDIR
> sbatch run_wrf.bash
---
Check wrf.slurm.out for run completion.
Also check wrf.rsl.out.<node> and wrf.rsl.error.<node> for
    tracking run failures or debugging.
```

Post-processing on Discover

Using NCVIEW:

```
WRF output files (NETCDF4) can be viewed using a special version
    of ncview installed on Discover:

/usr/local/other/SLES11/ncview/2.1.1/bin/ncview <filename>
```

Post-processing on Discover

Using RIP (NCAR graphics). Submit the **rip** job:

```
> cd $RUNDIR
> sbatch run_rip.bash # (or use sbatch)
> idt filename.cgm # Substitute actual filename

run_rip.bash will run ripdp_wrfarw and rip to generate NCAR
    Graphics cgm files.
idt is a NCAR Graphics executable in $NCARG_ROOT/bin
Sample RIP plot specification tables are in $NUWRFDIR/scripts/rip
     and are looped through by run_rip.bash

See http://www2.mmm.ucar.edu/wrf/users/docs/ripug.htm for info on
     customizing plots with RIP.
Minor changes to run_rip.bash may be necessary.
```

Post-processing on Discover

Other available community software packages are ARWPOST (for GRADS), UPP (for GRIB), and MET (for atmospheric verification)

For more information on community post-processing packages available with WRF, see

`http://www2.mmm.ucar.edu/wrf/users/docs/user_guide_V3.5/users_guide_chap9.htm`

ARW user homepage:

`http://www2.mmm.ucar.edu/wrf/users`

NUWRF specific post-processors are GSDSU (simulates satellite data) and LVT (land surface verification).

Adjustments for Pleiades

On Pleiades set PROJECTDIR to:

```
> export PROJECTDIR=/nobackupp8/nuwrf
```

Edit all the run* files for account information changes. If you belong to group s0492 then the scripts should work without any modifications.

```
Change s0942 to appropriate SBU charge code:
#PBS -W group_list=s0942
Change if you want to change number of nodes, "has" - to run on haswell nodes:
#PBS -l select=6:ncpus=16:mpiprocs=16:model=san
Uncomment and set according to your needs and privileges:
##PBS -q devel
Uncomment (if desired) and substitute your e-mail here:
##PBS -M=user@nasa.gov
```

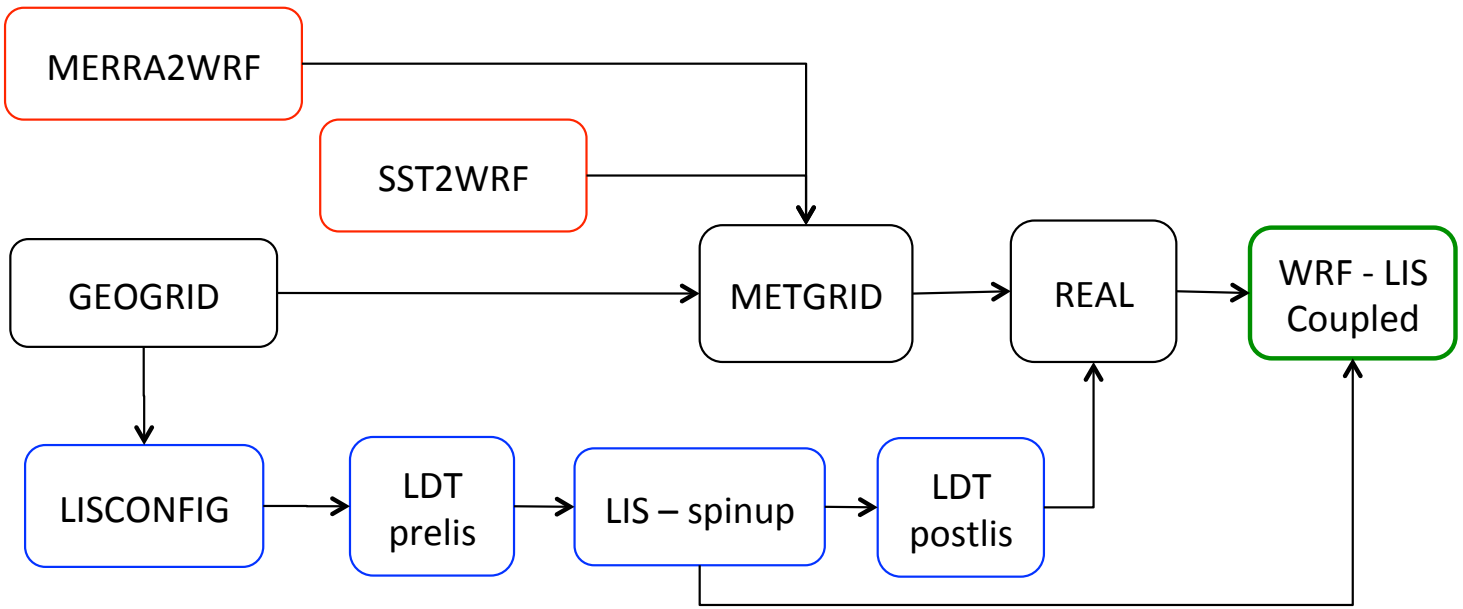
Default Workflow

The default workflow is a more advanced approach to running simulations with NU-WRF. Instead of using land surface fields interpolated from a coarser model or reanalysis, a custom-made land surface state is created by LIS on the same grid and with the same terrestrial data and land surface physics as WRF. WRF then calls LIS on each advective time step, and provides atmospheric forcing data and receives land surface data (fluxes, albedo, etc) in return.

No chemistry is used.

NU-WRF default workflow.

MERRA2WRF, SST2WRF, LIS spin up & WRF-LIS coupled workflow



This NU-WRF default workflow uses MERRA/ MERRA2 reanalysis atmospheric initial and lateral boundary conditions, RSS SST (Remote Sensing Systems SST product), and LIS land surface model initial conditions, and runs WRF coupled with LIS.

Required files for default workflow

Copy the following files to **RUNDIR**:

```
> cp -r $PROJECTDIR/tutorial/default $RUNDIR
```

```
Where:
common.cfg : shared script with settings used by other scripts.
run*.bash : scripts to run pre-processors and model.
namelist* : namelist files required by executables.
data/LIS_restarts: restarts used to run WRF with LIS.
```

Required script changes

```
> cd $RUNDIR
```

Use your favorite editor to edit **common.cfg** and change the values of NUWRFDIR and RUNDIR using the values set earlier.

```
# *** Please make sure these settings are correct ***
# NUWRFDIR specifies the location of the NU-WRF source code
NUWRFDIR=<CHANGE THIS>
# RUNDIR specifies the location of the temporary run directory
RUNDIR=<CHANGE THIS>
```

You may need to edit all the run* files' account information and other settings. However, if you belong to group s0492 then the scripts should work without any modifications.

```
Change account to appropriate SBU charge code:
#SBATCH --account s0942
Change if you want to change number of nodes, hasw - to run on haswell nodes:
#SBATCH --ntasks=16 --constraint=hasw
Uncomment and set according to your needs and privileges:
##SBATCH --qos=high
Uncomment (if desired) and substitute your e-mail here:
##SBATCH --mail-user=user@nasa.gov
```

A note about namelists settings

Things to keep in mind before we run NU-WRF components.

- The length of the simulations is specified in the namelist files:
  - In namelist.wps the length is determined by start_date and end_date
  - In namelist.input look for start_ and end_ fields.
  - The dates in both namelists must be consistent.
- The workflow is designed to work as-is. However, if you want to run for different dates:
  - You must get the corresponding atmospheric data for initial conditions.
  - Yo may need to modify the namelists. For example in namelist.input, make sure end_day - start_day = run_days.
- For **any** other changes please refer to the user's guide.

GEOGRID

GEOGRID interpolates static and climatological terrestrial data (land use, albedo, vegetation greenness, etc) to each WRF grid.

- Input: namelist.wps
- Output: For *N* domains (max_dom in namelist.wps), *N* geo_em files will be created.

To run:

```
> cd $RUNDIR
> sbatch run_geogrid.bash
---
When done, check for "Successful completion" string in the file
    geogrid.slurm.out. geogrid.log.<node> will also be created
    for tracking run failures or debugging.
```

Use of GEOS-5 Meteorological Data

Another source of NU-WRF initial and lateral boundary conditions is NASA's GEOS-5 global model. A number of dataset options exist from GEOS-5, including archived MERRA and MERRA-2 reanalyses. However, there are some issues to keep in mind.

First of all the GEOS-5 land surface data cannot be used to initialize WRF, due to fundamental differences between the GEOS-5 Catchment LSM and those in WRF. Thus, the GEOS-5 data in the current workflow also includes WRF-LIS. Second, GEOS-5 writes output in netCDF (and historically HDF4 and HDFEOS2) instead of GRIB. And furthermore, GEOS-5 often does not output all the variables expected by WPS.

To address these issues, special preprocessing software has been developed: MERRA2WRF. MERRA2WRF is a monolithic program customized to process the 6-hourly reanalyses from MERRA and MERRA-2. For 3-hourly MERRA-2 processing users must fall back to GEOS2WRF, which is not discussed here.

MERRA2WRF

MERRA2WRF scripts process the 6-hourly reanalyses from MERRA and MERRA-2. The scripts download data from the NASA GES DISC web servers. There are two cases - **for this tutorial we are doing case 2 below**:

Case 1: MERRA reanalysis for WRF initial and lateral boundary conditions.

```
> cd $RUNDIR
> cp $NUWRFDIR/utils/geos2wrf_2/scripts/run_merra/Run_MERRA.csh .
> ./Run_MERRA.csh 20070119 20070120 . $NUWRFDIR
> cp $RUNDIR/data/merra2wrf/MERRA* .
```

Case 2: MERRA2 reanalysis for WRF initial and lateral boundary conditions.

```
> cd $RUNDIR
> cp $NUWRFDIR/utils/geos2wrf_2/scripts/run_merra/Run_MERRA2.csh
    .
> ./Run_MERRA2.csh 20070119 20070120 . $NUWRFDIR
> cp $RUNDIR/data/merra2wrf/MERRA* $RUNDIR
```

SST2WRF

SST2WRF processes several sea surface temperature (SST) products produced by Remote Sensing Systems (RSS; see http://www.remss.com).

To run:

```
> cd $RUNDIR
> mkdir RUN_SST2WRF
> cd RUN_SST2WRF
> cp $NUWRFDIR/utils/sst2wrf/scripts/Run_SST.csh .

For a start date = 20070119 and end date = 20070120:

> ./Run_SST.csh 20070119 20070120 mw_ir . $NUWRFDIR

SSTRSS:* files will be created, and these files should be copied
    to the RUNDIR before running METGRID component.

> cp $RUNDIR/RUN_SST2WRF/sstdata/mw_ir/SSTRSS* $RUNDIR
```

METGRID

METGRID horizontally interpolates MERRA and SSTRSS data to the WRF domains, and combine them with the output from GEOGRID.

- Input: namelist.wps, MERRA*, SSTRSS* and geo_em* files.
- Output: Several met_em* files corresponding to number of intervals (interval_seconds) in simulation length (start/end dates).

To run:

```
> cd $RUNDIR
> sbatch run_metgrid.bash
---
When done, check for "Successful completion" string in the file
    metgrid.slurm.out. metgrid.log.<node> will also be created
    for tracking run failures or debugging.
```

LISCONFIG (optional step)

LISCONFIG is an optional utility for customizing LDT and LIS ASCII input files so their domain(s) (grid size, resolution, and map projection) match that of WRF. It uses the output from GEOGRID to determine the reference latitude and longitude. For this tutorial we are using pre-defined lis.config and ldt.config files, and the following steps are only shown for future reference.

- Input: lis.config, ldt.config and geo_em* files.
- Output: lis.config.new, ldt.config.new

To run:

```
> cd $RUNDIR
> cp $NUWRFDIR/utils/lisconfig/scripts/lisWrfDomain.py .
> ln -s $NUWRFDIR/utils/bin/lisWrfDomain.x ./EXE
> lisWrfDomain.py EXE lis.config ldt.config ./
```

LDT (pre-LIS)

LDT processes data inputs for different surface models. In this use-case we are using the Noah v3.6 land surface model.

- Input: ldt.config (ldt.config.prelis gets copied into ldt.config by run_ldt_prelis.bash)
- Output: lis_input* files for each NU-WRF domain.

To run:

```
> cd $RUNDIR
> sbatch run_ldt_prelis.bash
---
When done, check for "Finished LDT run" string in the file
    ldt_log_prelis.0000
```

LIS

LIS can be run in various modes. Here we run in "retrospective" mode and provide restart files as input to LIS (in data/LIS_restarts).

- Input: lis.config, LIS_RST_NOAH36*nc, forcing_variables_wrfcplmode.txt, NOAH36_OUTPUT_LIST_SPINUP.TBL
- Output: surface model output in OUTPUT directory.

To run:

```
> cd $RUNDIR
> sbatch run_lis.bash
---
Check this file for successful run completion: lis.slurm.out
lislog.<node> will also be created for tracking run failures or
    debugging.
```

For more information about LIS see

https://modelingguru.nasa.gov/community/atmospheric/lis.

LDT (post-LIS)

After running LIS, it is necessary to rerun LDT in "NUWRF preprocessing for real" mode. This requires modifications to ldt.config to specify the static output file from LDT and the dynamic output file from LIS. Fields from both will be combined and written to a new netCDF output file for use by REAL

- Input: ldt.config (ldt.config.postlis gets copied into ldt.config by run_ldt_postlis.bash), LIS history files in OUTPUT directory.
- Output: lis4real_input* files for each NU-WRF domain.

To run:

```
> cd $RUNDIR
> sbatch run_ldt_prelis.bash
---
When done, check for "Finished LDT run" string in the file
    ldt_log_postlis.0000
```

REAL

REAL vertically interpolates the METGRID output to the WRF grid, and creates initial and lateral boundary condition files.

- Input: namelist.input, met_em* files, geo_em*, lis4real_input* files.
- Output: wrfinput* files (one for each domain), wrfbdy_d01.

To run:

```
> cd $RUNDIR
> sbatch run_real.bash
---
Check real.slurm.out for run completion.
Also check real.rsl.out.<node> and real.rsl.error.<node> for
    tracking run failures or debugging.
```

WRF

Running WRF in this case is similar to the basic case, except that WRF will also read the lis.config file and the LIS restart files that were produced during the "retrospective" run.

- Input: wrfinput* files (one for each domain), wrfbdy_d01.
- Output: wrfout* and wrfrst* files (one for each domain).

To run:

```
> cd $RUNDIR
> cp namelist.input.wrf namelist.input
> cp lis.config.wrflis lis.config
> sbatch run_wrf.bash
---
Check wrf.slurm.out for run completion.
Also check wrf.rsl.out.<node> and wrf.rsl.error.<node> for
    tracking run failures/ debugging.
```

Post-processing on Discover

Using NCVIEW:

```
WRF output files (NETCDF4) can be viewed using a special version
    of ncview installed on Discover:

/usr/local/other/SLES11/ncview/2.1.1/bin/ncview <filename>
```

Post-processing on Discover

Using RIP (NCAR graphics). Submit the **rip** job:

```
> cd $RUNDIR
> sbatch run_rip.bash # (or use sbatch)
> idt filename.cgm # Substitute actual filename

run_rip.bash will run ripdp_wrfarw and rip to generate NCAR
    Graphics cgm files.
idt is a NCAR Graphics executable in $NCARG_ROOT/bin
Sample RIP plot specification tables are in $NUWRFDIR/scripts/rip
     and are looped through by run_rip.bash

See http://www2.mmm.ucar.edu/wrf/users/docs/ripug.htm for info on
     customizing plots with RIP.
Minor changes to run_rip.bash may be necessary.
```

Chemistry Workflow

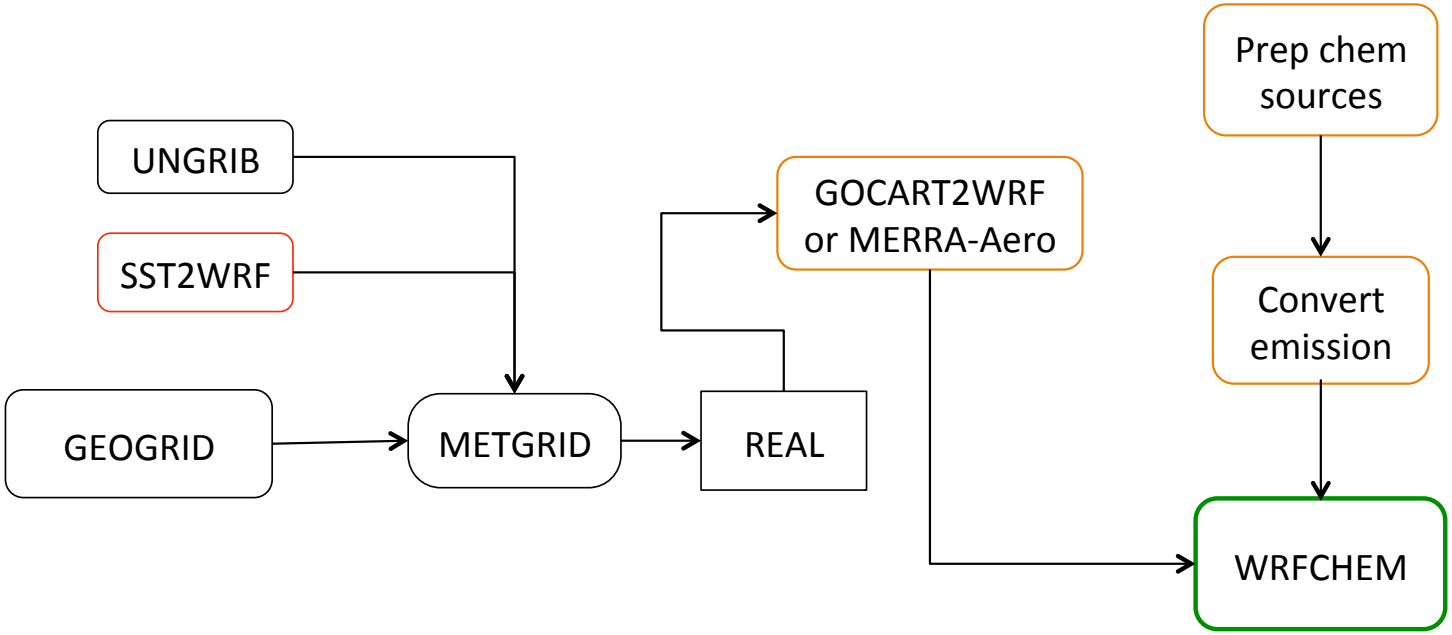
NU-WRF offers advanced aerosol modeling using the implementation of GOCART. This workflow is similar to the default workflow but excludes the LIS steps and instead adds the GOCART2WRF preprocessor for providing chemical boundary conditions from GEOS-5 as well as the community PREP_CHEM_SOURCES program for emissions.

GOCART2WRF supports four possible sources of GOCART data:

- offline GOCART
- on-line GOCART from GEOS5
- MERRAero reanalyses
- MERRA-2

We will describe the "offline GOCART" case only.
LIS is not used.

NU-WRF chemistry workflow.



This NU-WRF CHEM workflow uses atmospheric initial and lateral boundary conditions from GRIB files, RSS SST (Remote Sensing Systems SST product), and chemical tracers using Prep-chem sources, Convert_emiss, aerosol data from GOCART or MERRA-Aero, and runs WRF-CHEM.

Required files for chemistry workflow

Copy the following files to **RUNDIR**:

```
> cp -r $PROJECTDIR/tutorial/chemistry $RUNDIR
```

```
Where:
common.cfg : shared script with settings used by other scripts.
run*.bash : scripts to run pre-processors, model and post-
    processor.
namelist* : namelist files required by executables.
data/ungrib : GRIB atmospheric data for initial conditions used
    by UNGRIB component.
data/gocart : data files used by GOCART
```

Required script changes

```
> cd $RUNDIR
```

Use your favorite editor to edit **common.cfg** and change the values of NUWRFDIR and RUNDIR using the values set earlier.

```
# *** Please make sure these settings are correct ***
# NUWRFDIR specifies the location of the NU-WRF source code
NUWRFDIR=<CHANGE THIS>
# RUNDIR specifies the location of the temporary run directory
RUNDIR=<CHANGE THIS>
```

You may need to edit all the run* files' account information and other settings. However, if you belong to group s0492 then the scripts should work without any modifications.

```
Change account to appropriate SBU charge code:
#SBATCH --account s0942
Change if you want to change number of nodes, hasw - to run on haswell nodes:
#SBATCH --ntasks=16 --constraint=hasw
Uncomment and set according to your needs and privileges:
##SBATCH --qos=high
Uncomment (if desired) and substitute your e-mail here:
##SBATCH --mail-user=user@nasa.gov
```

A note about namelists settings

Things to keep in mind before we run NU-WRF components.

- The length of the simulations is specified in the namelist files:
  - In namelist.wps the length is determined by start_date and end_date
  - In namelist.input look for start_ and end_ fields.
  - The dates in both namelists must be consistent.
- The workflow is designed to work as-is. However, if you want to run for different dates:
  - You must get the corresponding atmospheric data for initial conditions.
  - Yo may need to modify the namelists. For example in namelist.input, make sure end_day - start_day = run_days.
- For **any** other changes please refer to the user's guide.

GEOGRID

GEOGRID interpolates static and climatological terrestrial data (land use, albedo, vegetation greenness, etc) to each WRF grid.

- Input: namelist.wps
- Output: For *N* domains (max_dom in namelist.wps), *N* geo_em files will be created.

To run:

```
> cd $RUNDIR
> sbatch run_geogrid.bash
---
When done, check for "Successful completion" string in the file
    geogrid.slurm.out. geogrid.log.<node> will also be created
    for tracking run failures or debugging.
```

UNGRIB

UNGRIB reads GRIB or GRIB2 files with dynamic meteorological and dynamic terrestrial data (soil moisture, soil temperature, sea surface temperature, sea ice, etc) and write specific fields in WPS intermediate format.

- Input: namelist.wps. Important fields are interval_seconds and start/end dates.
- Output: Several NAM* files corresponding to number of intervals (interval_seconds) in simulation length (start/end dates).

NOTE: The GRIB input is referenced in the run script, run_ungrib.bash:
./link_grib.csh data/ungrib/*
The UNGRIB output (NAM) is determined by the settings in the WPS namelist (namelist.wps).

To run:

```
> cd $RUNDIR
> ./run_ungrib.bash
---
When done, check for "Successful completion" string in the file
    ungrib.slurm.out. ungrib.log will also be created for
    tracking run failures or debugging.
```

SST2WRF

SST2WRF processes several sea surface temperature (SST) products produced by Remote Sensing Systems (RSS; see http://www.remss.com).

To run:

```
> cd $RUNDIR
> mkdir RUN_SST2WRF
> cd RUN_SST2WRF
> cp $NUWRFDIR/utils/sst2wrf/scripts/Run_SST.csh .

For the specified (in namelist.wps) start date = 20090410 and end
     date of 20090411:

> ./Run_SST.csh 20090410 20090411 mw_ir . $NUWRFDIR

SSTRSS:* files will be created, and these files should be copied
    to the RUNDIR before running METGRID component.

> cp $RUNDIR/RUN_SST2WRF/sstdata/mw_ir/SSTRSS* $RUNDIR
```

METGRID

METGRID horizontally interpolates UNGRIB and SSTRSS output to the WRF domains, and combine them with the output from GEOGRID.

- Input: namelist.wps, geo_em*, NAM*, and SSTRSS* files.
- Output: Several met_em* files corresponding to number of intervals (interval_seconds) in simulation length (start/end dates).

To run:

```
> cd $RUNDIR
> sbatch run_metgrid.bash
---
When done, check for "Successful completion" string in the file
    metgrid.slurm.out. metgrid.log.<node> will also be created
    for tracking run failures or debugging.
```

REAL

REAL vertically interpolates the METGRID output to the WRF grid, and creates initial and lateral boundary condition files.

- Input: namelist.input, met_em* files.
- Output: wrfinput* files (one for each domain), wrfbdy_d01.

To run:

```
> cd $RUNDIR
> sbatch run_real.bash
---
Check real.slurm.out for run completion.
Also check real.rsl.out.<node> and real.rsl.error.<node> for
    tracking run failures or debugging.
```

GOCART2WRF

GOCART2WRF extracts aerosol data from GEOS-5 netCDF4 GOCART files (or MERRA reanalysis aerosol data files); horizontally and vertically interpolates the fields to the WRF grid; and appends them to the initial and lateral boundary condition files of WRF (wrfinput_d* and wrfbdy_d01).
User can choose GOCART aerosol data or MERRA reanalysis Aerosol data.

- Input: namelist.gocart2wrf, grib_input/*, wrfinput* files (one for each domain), wrfbdy_d01.
- Output: wrfinput* files (one for each domain), wrfbdy_d01. Original wrfinput* and wrfbdy_d01 files will be backed up with .gocart2wrf extension.

To run:

```
> cd $RUNDIR
>./run_gocart2wrf.bash # runs in serial
---
Check this file for successful run completion: gc2wrf.log.
```

PREP_CHEM_SOURCES

This community tool processes a number of biogenic, anthropogenic, volcanic, and wildfire emissions. The NU-WRF version has several modifications that are discussed in the user's guide. Running prep_chem_sources requires a prep_chem_sources.inp file and upon completion it produces map projection data (that can be visualized by plot_chem) as well as other files used by convert_emiss.

- Input: prep_chem_sources.inp
- Output: nuwrf-T* files

To run:

```
> cd $RUNDIR
> ./run_prep_chem_sources.bash
---
Check this file for successful run completion: pcs.log.
```

Convert_Emiss

This is a community WRF-Chem preprocessor that takes the output from PREP CHEM SOURCES and rewrites the fields in new netCDF files for reading by WRF-Chem.

- Input: namelist.input.convert_emiss files (one for each domain).
- Output: wrfchemi_gocart_bg* and wrfchemi* files (one for each domain).

To run:

```
> cd $RUNDIR
> sbatch run_convert_emiss.bash
---
Check ce.slurm.out for run completion.
```

WRF

If we get to this point then we are ready to run WRF with chemistry.

- Input: wrfinput* files (one for each domain), wrfbdy_d01, wrfchemi_gocart_bg* and wrfchemi* files.
- Output: wrfout* and wrfrst* files (one for each domain).

To run:

```
> cd $RUNDIR
> sbatch run_wrf.bash
---
Check wrf.slurm.out for run completion. Also check wrf.rsl.out.<
    node> and wrf.rsl.error.<node> for tracking run failures/
    debugging.
```

Post-processing on Discover

Using NCVIEW:

```
WRF output files (NETCDF4) can be viewed using a special version
    of ncview installed on Discover:

/usr/local/other/SLES11/ncview/2.1.1/bin/ncview <filename>
```

Post-processing on Discover

Using RIP (NCAR graphics). Submit the **rip** job:

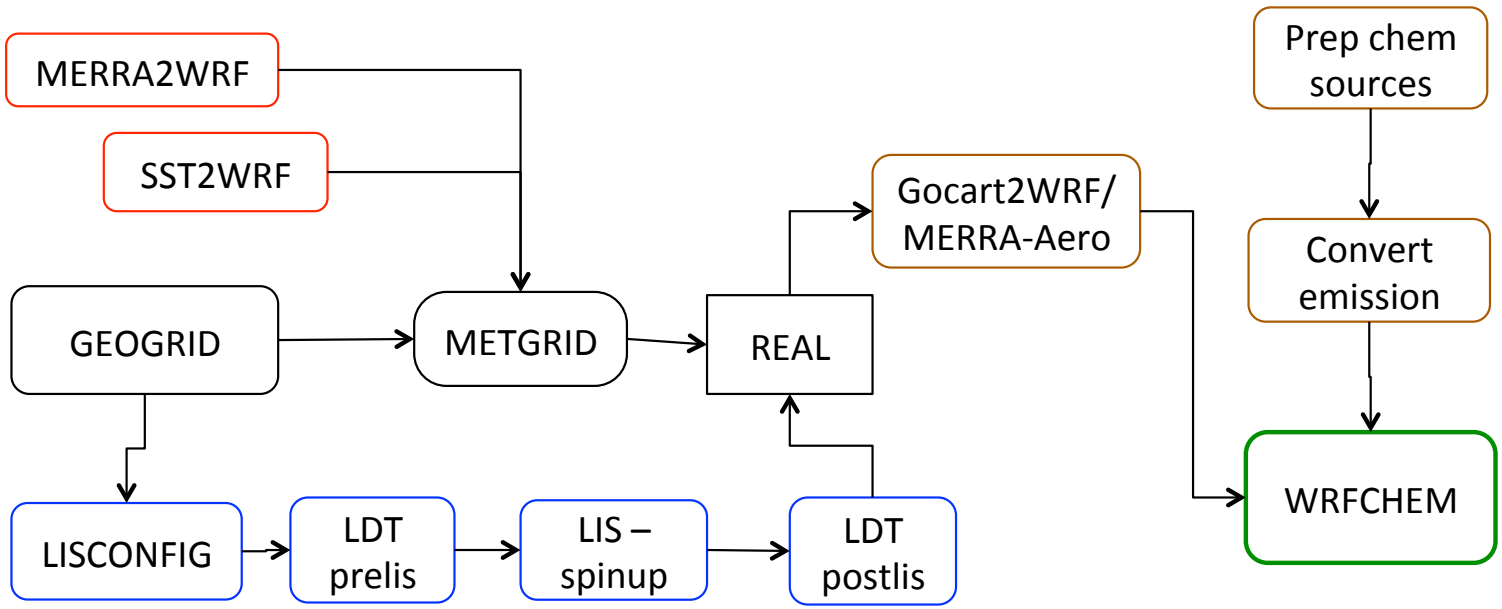
```
> cd $RUNDIR
>  run_rip.bash # (or use sbatch)
> idt filename.cgm # Substitute actual filename

run_rip.bash will run ripdp_wrfarw and rip to generate NCAR
    Graphics cgm files.
idt is a NCAR Graphics executable in $NCARG_ROOT/bin
Sample RIP plot specification tables are in $NUWRFDIR/scripts/rip
     and are looped through by run_rip.bash

See http://www2.mmm.ucar.edu/wrf/users/docs/ripug.htm for info on
     customizing plots with RIP.
Minor changes to run_rip.bash may be necessary.
```

The workflow just described can be modified to use MERRA/ MERRA2 reanalysis atmospheric initial and lateral boundary conditions, RSS SST (Remote Sensing Sytems SST product) along with LIS land surface model initial conditions (see diagram in the next page). Just replace the UNGRIB step by the MERRA2WRF step and add the LDT-LIS-LDT steps before running REAL.

Alternate NU-WRF chemistry workflow.



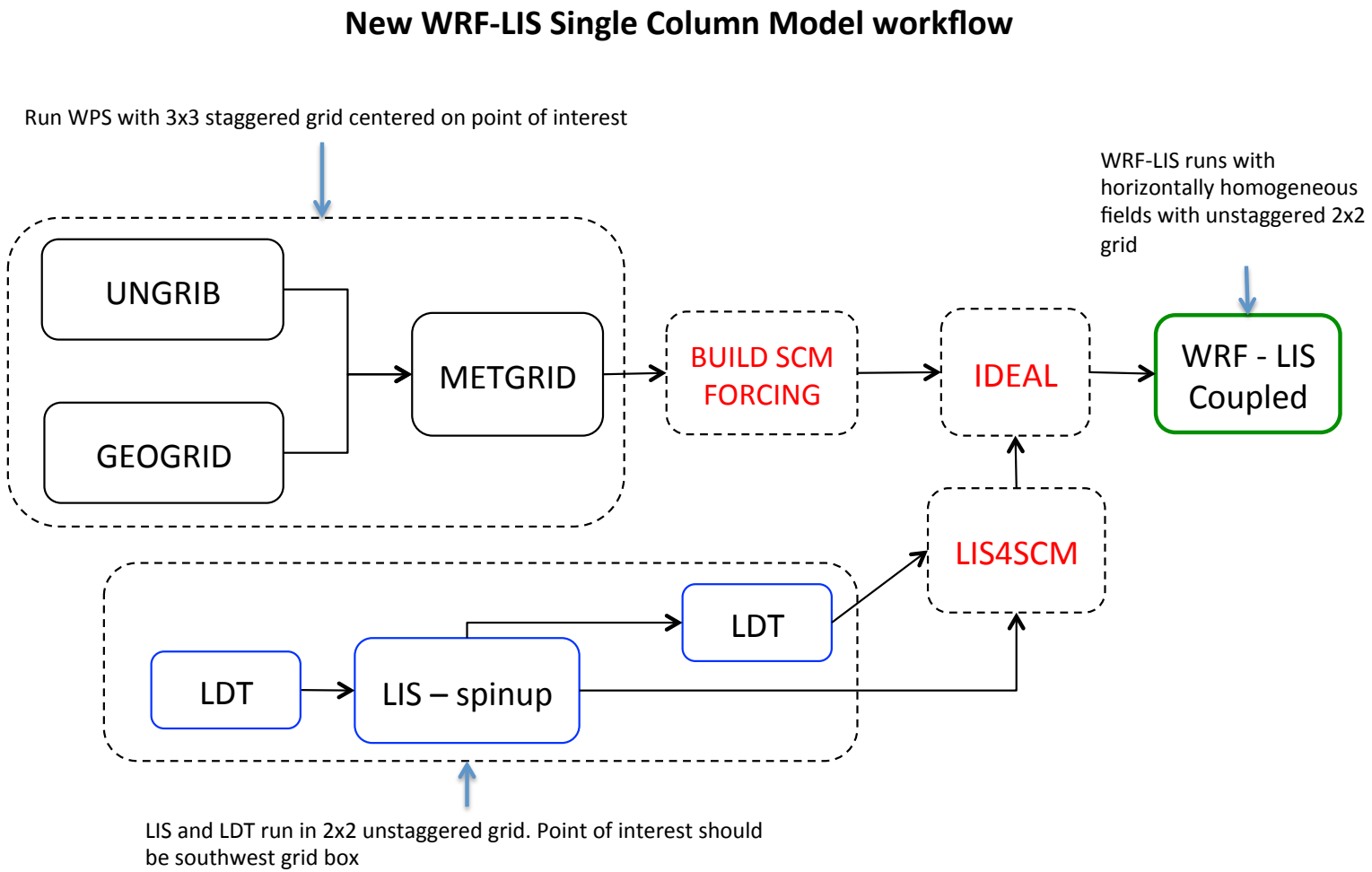
This NU-WRF-CHEM workflow uses MERRA/ MERRA2 reanalysis atmospheric initial and lateral boundary conditions, RSS SST (Remote Sensing Sytems SST product) along with LIS land surface model initial conditions, and other chemical tracers from Prep-chem sources, and runs WRF-CHEM.

SCM Workflow

The SCM workflow describes the steps necessary to setup and run WRF-LIS (like the default workflow) using a single point domain.

No chemistry is used.

NU-WRF Single Column Model (SCM) workflow.



Required files for SCM workflow

Copy the following files to **RUNDIR**:

```
> cd $RUNDIR
> cp $PROJECTDIR/tutorial/scm/*.* .
> cp -r $PROJECTDIR/tutorial/scm/data/ungrib ungrib_input
```

Where:

common.cfg : shared script with settings used by other scripts.
run*.bash : scripts to run pre-processors and model.
namelist* : namelist files required by executables.

Required script changes

```
> cd $RUNDIR
```

Use your favorite editor to edit **common.cfg** and change the values of NUWRFDIR and RUNDIR using the values set earlier.

```
# *** Please make sure these settings are correct ***
# NUWRFDIR specifies the location of the NU-WRF source code
NUWRFDIR=<CHANGE THIS>
# RUNDIR specifies the location of the temporary run directory
RUNDIR=<CHANGE THIS>
```

You may need to edit all the run* files' account information and other settings. However, if you belong to group s0492 then the scripts should work without any modifications.

```
Change account to appropriate SBU charge code:
#SBATCH --account s0942
The SCM runs on 1 CPU only. Do not change --ntasks to any other value!
#SBATCH --ntasks=1
Most SCM runs are very short, so use debug queue if possible.
##SBATCH --qos=debug
Uncomment (if desired) and substitute your e-mail here:
##SBATCH --mail-user=user@nasa.gov
```

A note about namelists settings

Things to keep in mind before we run NU-WRF components.

- The length of the simulations is specified in the namelist files:
  - In namelist.wps the length is determined by start_date and end_date
  - In namelist.input look for start_ and end_ fields.
  - The dates in both namelists must be consistent.
- The workflow is designed to work as-is. However, if you want to run for different dates:
  - You must get the corresponding atmospheric data for initial conditions.
  - Yo may need to modify the namelists. For example in namelist.input, make sure end_day - start_day = run_days.
- For **any** other changes please refer to the user's guide.

GEOGRID

GEOGRID interpolates static and climatological terrestrial data (land use, albedo, vegetation greenness, etc) to each WRF grid.

- Input: namelist.wps
- Output: For *N* domains (max_dom in namelist.wps), *N* geo_em files will be created.

To run:

```
> cd $RUNDIR
> sbatch run_geogrid.bash
---
When done, check for "Successful completion" string in the file
    geogrid.slurm.out. geogrid.log.<node> will also be created
    for tracking run failures or debugging.
```

UNGRIB

UNGRIB reads GRIB or GRIB2 files with dynamic meteorological and dynamic terrestrial data (soil moisture, soil temperature, sea surface temperature, sea ice, etc) and writes specific fields in a WPS intermediate format.

- Input: namelist.wps, ungrib_input/* files.
- Output: NARR* files.

NOTE: The GRIB input is referenced in the run script, run_ungrib.bash:
./link_grib.csh ungrib_input/*
The UNGRIB output (NARR) is determined by the settings in the WPS namelist (namelist.wps).

To run:

```
> cd $RUNDIR
> sbatch run_ungrib.bash
---
When done, check for "Successful completion" string in the file
    ungrib.slurm.out. ungrib.log will also be created for
    tracking run failures or debugging.
```

METGRID

METGRID horizontally interpolates the output from UNGRIB to the WRF domains, and combines it with the output from GEOGRID.

- Input: namelist.wps, NARR* files, geo_em* files.
- Output: Several met_em* files corresponding to number of intervals (interval_seconds) in simulation length (start/end dates).

To run:

```
> cd $RUNDIR
> sbatch run_metgrid.bash
---
When done, check for "Successful completion" string in the file
    metgrid.slurm.out. metgrid.log.<node> will also be created
    for tracking run failures or debugging.
```

BUILD_SCM_FORCING

BUILD_SCM_FORCING scripts use WPS output and generate column initial conditions profile_init.txt and surface_init.txt.
Note that this script depends on NCL and on Discover one needs to load other/ncl-6.3.0-static.

- Input: WPS output, forcing_file.cdl and several *.ncl files.
- Output: profile_init.txt, surface_init.txt, and a directory, 2006-07-14_00:00:00, containing forcing_file.nc and input_sounding data.

To run:

```
> cd $RUNDIR

Edit build_scm_forcing.bash: set metPath and forceArcRoot equal
    to RUNDIR value.

> build_scm_forcing.bash # runs in serial
```

LDT (pre-LIS)

LDT processes data inputs for different surface models. In this use-case we are using the Noah v3.6 land surface model.

- Input: ldt.config
- Output: lis_input* files for each NU-WRF domain.

To run:

```
> cd $RUNDIR
> sbatch run_ldt_prelis.bash
---
When done, check for "Finished LDT run" string in the file
    ldt_log_prelis.0000
```

LIS

LIS can be run from a cold start or from a restart. A cold start run is usually a multi-year simulation, not appropriate for a tutorial. In the restart case we have to provide restart files as input (LIS_RST* files) and LIS run is significantly shorter. Nevertheless, the restart files have already been generated for this tutorial and the user can **skip** this step.

- Input: lis.config, LIS_RST_NOAH36*nc, forcing_variables_wrfcplmode.txt, NOAH36_OUTPUT_LIST_SPINUP.TBL
- Output: LIS_RST_NOAH36*nc files, one for each NU-WRF domain.

To run:

```
> cd $RUNDIR
> sbatch run_lis.bash
---
Check this file for successful run completion: lis.slurm.out
lislog.<node> will also be created for tracking run failures or
    debugging.
```

LDT (post-LIS)

After running LIS, it is necessary to rerun LDT in "NUWRF preprocessing for real" mode. This requires modifications to ldt.config to specify the static output file from LDT and the dynamic output file from LIS. Fields from both will be combined and written to a new netCDF output file for use by REAL

- Input: ldt.config
- Output: lis4real_input* files for each NU-WRF domain.

To run:

```
> cd $RUNDIR
> sbatch run_ldt_postlis.bash
---
When done, check for "Finished LDT run" string in the file
    ldt_log_postlis.0000
```

LIS4SCM

LIS4SCM copies data from southwest grid point to remainder of LIS/LDT domain (becomes horizontally homogenous): LIS4SCM imposes identical lat/lon at each LIS point in the restart file.

- Input: namelist.lis4scm, LDT-LIS-LDT output
- Output: Horizontally homogeneous lis_input file.

To run:

```
> cd $RUNDIR
> ./run_lis4scm.bash # Note this runs in serial
```

IDEAL

IDEAL creates wrfinput file from text column data and homogeneous LIS/LDT file.

- Input: LIS4SCM output
- Output: wrfinput file.

To run:

```
> cd $RUNDIR
> cp 2006-07-14_00:00:00/* .
> sbatch run_ideal.bash
```

WRF-LIS

WRF-LIS reads wrfinput and homogenous LIS restart file.

- Input: wrfinput file
- Output: wrfoutput file.

To run:

```
> cd $RUNDIR
> sbatch run_wrf.bash
```

Notes:

- Tested case uses periodic LBCs (thus, no wrfbdy file).
- Tested case also used no forcing (no external advection, etc).
- Tested case used dx = 1 km, dt = 6 sec (runs very fast!)

Post-processing on Discover

Using NCVIEW:

```
WRF output files (NETCDF4) can be viewed using a special version
    of ncview installed on Discover:

/usr/local/other/SLES11/ncview/2.1.1/bin/ncview <filename>
```

Post-processing on Discover

Using RIP (NCAR graphics). Submit the **rip** job:

```
> cd $RUNDIR
>  run_rip.bash # (or use sbatch)
> idt filename.cgm # Substitute actual filename

run_rip.bash will run ripdp_wrfarw and rip to generate NCAR
    Graphics cgm files.
idt is a NCAR Graphics executable in $NCARG_ROOT/bin
Sample RIP plot specification tables are in $NUWRFDIR/scripts/rip
     and are looped through by run_rip.bash

See http://www2.mmm.ucar.edu/wrf/users/docs/ripug.htm for info on
     customizing plots with RIP.
Minor changes to run_rip.bash may be necessary.
```

Regression testing

Definition

From Wikipedia:

```
Regression testing is a type of software testing that verifies that
software previously developed and tested still performs correctly
even after it was changed or interfaced with other software.
Changes may include software enhancements, patches,
configuration changes, etc. During regression  testing, new
software bugs or regressions may be uncovered.
```

Testing types

Software testing can be roughly divided into three categories:

- Automated regression tests. These tests compile and run a very large number of model configurations and may perform various checks.
- Manual/user testing. These tests are intended to be performed by users that wish to verify their changes prior to pushing to a central repository. In detail, these tests are similar to the automated tests, but are more easily executed from the command line.
- Unit tests. These tests execute extremely quickly and provide a finer-grained verification than the other regression tests, albeit with far less coverage of the source code. *Unit tests do not form part of the NU-WRF code base at this time*.

In this section we discuss the available NU-WRF regression testing infrastructure and how it can be used to perform automated and manual tests.

NU-WRF regression testing scripts

The NU-WRF regression scripts are a set of python scripts and configuration files designed to run tests on the NU-WRF code base. The scripts' functionality is all driven by the settings specified in a single configuration file.

The configuration file is a text file with a particular structure readable by the python scripts and easily understood by humans too! The files are organized into sections, and each section contains name-value pairs for configuration data.

NU-WRF regression testing scripts

There is one configuration file required by the scripts - specified as a command line argument. The file can have any name but must have the '.cfg' extension. A sample configuration file (sample.cfg) is included $NUWRFDIR/scripts/regression that can be used for "routine" testing.

Note:

There are three additional files that are used specifically for NU-WRF testing: master.cfg, develop.cfg and comp.cfg. These files should not be modified or used for anything other than as reference to build your own customized configuration.

Workflows revisited

In this document we have discussed 4 workflows: basic, default, chemistry and scm. For the purposes of regression testing workflows are categorized as follows:

- wrf: default WRF-ARW runs (without LIS) (basic)
- wrflis: like wrf but with LIS-coupling (default and scm)
- chem: like wrf with chemistry (chemistry)
- kpp: like wrf with chemistry - uses KPP (chemistry)

This distinction is necessary to specify test cases in the configuration file. For a list of all supported NU-WRF configurations see:

$NUWRFDIR/scripts/regression/master.cfg

Python scripts

The python scripts are the following:

- reg : Main driver.
- RegPool.py : A class with functionality to parallelize tasks.
- regression.py : A driver script to execute the NU-WRF component tasks.
- RegRuns.py : A class that defines regression test run instances.
- RegTest.py : A class that defines regression test instances.
- reg_tools.py : Various tools used by the main drivers.
- reg_utils.py : Various utilities used by all the scripts.

The scripts can be used to perform both automated regression tests as well as "manual testing".

Manual testing

Before running the regression testing scripts make sure you duplicate the sample.cfg file and customize it to your needs. When ready to run the scripts, specify the configuration file name as an argument to reg and wait for the results:

```
$ cd $NUWRFDIR/scripts/regression

To run the scripts, specify the configuration file name as an
argument to reg:

$ reg <cfg_file> &

Note that the extension should not be specified.
```

Manual testing

Upon execution you will see some messages echoed to STDOUT
but all the output will be logged to a file named <cfg_file>.LOG.

There will be other "log" files, one for each <workflow> and one for each <experiment>, that will be generated for each 'reg' run.

Workflow builds, a maximum of four, will be generated in <scratch_dir>/builds

Each build will have its own make.log as well as <workflow>.out and <wo files that will be useful to diagnose build errors.

Manual testing

Run logs will be generated in each run directory under <scratch_dir>/results.
These will have the name <experiment>-regression.log
and should also be very useful to diagnose test-case-specific run-time issues.

At the end of a "reg" an email test report will be emailed to the recipient specified in the mail_to field in USERCONFIG.

Note that all 'reg' runs are tagged with a unique time stamp corresponding to the date/time the run was executed.

Manual testing within interactive queue

One can run NU-WRF test cases interactively. To do so make sure you set use_batch=no in your configuration file. Also, if running interactively, one can only use one compiler option; i.e. in the 'compilers' setting you can only use intel-sgimpt or gnu-mvapich2. With those caveats in mind:

```
Request an interactive queue on DISCOVER, for example:

salloc --ntasks=84 --time=1:00:00 --account=s0492 --constraint=hasw

Once you get the prompt

$ cd $NUWRFDIR/scripts/regression

$ reg <cfg_file> &

Note that the extension should not be specified.
```

As you may have figured out, all the workflows described earlier in this tutorial can be recreated with the appropriate configuration file and the testing scripts.

For more information about regression testing or any workflow described in this tutorial please feel free to contact any member of the NU-WRF software integration group.